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HIGH PRODUCTION VOLUME (HPV)

CHEMICAL CHALLENGE PROGRAM

TEST PLAN

For

Phenol, Heptyl Derivatives

Prepared by
The American Chemistry Council
Petroleum Additives Panel
Health, Environmental, and Regulatory Task Group

December 2003

**LIST OF MEMBER COMPANIES IN THE
HEALTH, ENVIRONMENTAL AND REGULATORY TASK GROUP**

The Health, Environmental, and Regulatory Task Group (HERTG) of the American Chemistry Council Petroleum Additives Panel includes the following member companies:

Chevron Oronite Company, LLC

Crompton Corporation

Ethyl Corporation

ExxonMobil Chemical Company

Ferro Corporation

Groupe SNPE

Infineum

The Lubrizol Corporation

Rhein Chemie Corporation

Rhodia, Inc.

1.0 INTRODUCTION

In March 1999, the American Chemistry Council (formerly the Chemical Manufacturers Association) Petroleum Additives Panel Health, Environmental, and Regulatory Task Group (HERTG), and its participating member companies committed to address data needs for certain chemicals listed under the Environmental Protection Agency (EPA) High Production Volume (HPV) Chemical Challenge Program. This test plan follows up on that commitment. Specifically, this test plan sets forth how the HERTG intends to address testing information for the following substance - phenol, heptyl derivatives (CAS No.: 72624-02-3).

In preparing this test plan the following steps were undertaken:

> Step 1: A review of the literature and confidential company data was conducted on the physicochemical properties, mammalian toxicity endpoints, and environmental fate and effects for phenol, heptyl derivatives, using its CAS number, CAS name, and synonyms. Searches included the following sources: MEDLINE, BIOSIS, CANCERLIT, CAPLUS, CHEMLIST, EMBASE, HSDB, RTECS, EMIC, TOXLINE, TSCATS databases as well as standard handbooks and databases (e.g., Sax, CRC Handbook on Chemicals, IUCLID, Merck Index).
>
> Step 2: The compiled data was evaluated for adequacy in accordance with the EPA guidance documentation.

Prior to initiation of the testing proposed in this test plan, the HERTG will review any relevant data available on similar alkyl phenol test plans submitted under the HPV Challenge Program for possible inclusion of that data in this test plan.

2.0 GENERAL SUBSTANCE INFORMATION

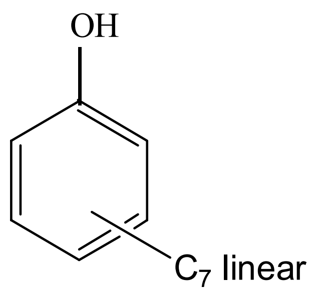
The substance that is the subject of this test plan is used as a precursor molecule in the manufacture of petroleum additives used in highly refined lubricating base oil. The chemical name, CAS Registry Number, molecular weight and chemical structure for this substance are presented below.

Chemical Name: Phenol, heptyl derivatives

Chemical Abstract Service Registry Number: 72624-02-3
Alternative Chemical Abstract Service Registry Number: 1987-50-4

Molecular Weight**:** 192.3 gm/mol

Chemical Structure:

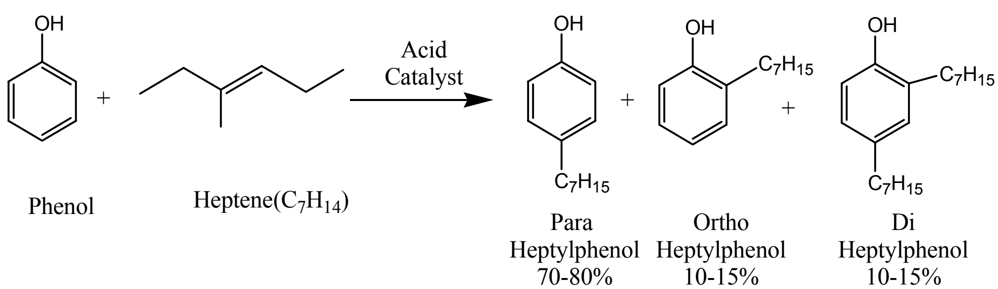


72624-02-3

3.0 EXPOSURE INFORMATION

Manufacture: Phenol, heptyl derivatives (HPL) is made through the acid-catalyzed alkylation of phenol with industrial grade heptenes. The heptenes used to make HPL are a complex mixture of branched isomers obtained from the acid catalyzed polymerization of propylene–butylene mixtures. The general reaction process is shown in Figure 1, together with the typical levels of the major components.

Figure 1



Based on supplier information, HPL has a relatively narrow homolog distribution, where C7 alkylphenol comprises greater than 95% of the total olefins in the mixture. No significant contaminates or by-products are present, and combined levels of unreacted heptene and phenol are generally less than 1% of the total mixture.

Use in Lubricants: The principal use of HPL is as a building block to manufacture higher molecular weight oligomeric lubricating additive components. These components are highly stable and not expected to release HPL under normal use in these applications. The level of unreacted HPL in these products is less than 1%.

HPL is used to manufacture a variety of lubricant additives. These additives are typically blended with other additives into lubricant concentrates, which are then sold to lubricant marketers who then blend them with oil and, in some cases, additional additives, to yield the final (finished) lubricant. This finished lubricant is then sold to the end user for use in the lubricant application.

The additives derived from HPL are used as detergents and metal deactivators in a wide variety of lubricating applications including industrial and automotive gear oils, automatic transmission formulations, and small engine applications. The average level of unreacted HPL in these finished lubricants is estimated to be very low.

4.0 PHYSICOCHEMICAL PROPERTIES

4.1 Summary of Available Data

4.1.1 Melting Point

Heptylphenol is a liquid at ambient temperature. The freezing point of heptylphenol is < -5°C (Product data sheet – Schenectady International Inc.).

4.1.2 Boiling Point

The boiling point range of heptylphenol is 256 – 280°C (Product data sheet – Schenectady International Inc).

4.1.3 Vapor Pressure

The vapor pressure of heptylphenol is 0.0113 mmHg @ 25°C (Product data sheet – Schenectady International Inc).

4.1.4 Water Solubility

The water solubility of heptylphenol is 12.2 mg/L as measured by the shake flask method (Product data sheet – Schenectady International Inc).

4.1.5 Octanol/Water Partition Coefficient

The log octanol/water partition coefficient of heptylphenol has been estimated at 4.5 (Tollefsen et al[1].)

5.0 ENVIRONMENTAL FATE DATA

5.1 Biodegradability

5.1.1 Summary of Available Data

Phenol, heptyl derivatives are not readily biodegradable.

5.1.2 Data Assessment and Test Plan for Biodegradability

An adequate and reliable biodegradation test has been conducted on phenol, heptyl derivatives according to OECD Test Guideline 301B and ASTM D5864 guidelines using adapted inoculum. The results indicate that this material is inherently biodegradable based on a degradation of 25% after 28 days. In addition to above,

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[1] Tollefsen et al. Acute Toxicity and Toxicokinetics of 4-Heptyl phenol in Juvenile Atlantic Cod (Gadus Morhua L.). Environmental Toxicology and Chemistry Vol 17, No. 4. pp. 740-746. 1998.

studies available in the literature[2] indicate approximately 40% biodegradation in seawater over 28-days. Additional biodegradation testing is not proposed.

5.2 Hydrolysis

5.2.1 Summary of Available Data

No published or unpublished hydrolysis studies with phenol, heptyl derivatives were located.

5.2.2 Data Assessment and Test Plan for Hydrolysis

Hydrolysis of an organic chemical is the transformation process in which a water molecule or hydroxide ion reacts to form a new carbon-oxygen bond. Chemicals that have a potential to hydrolyze include alkyl halides, amides, carbamates, carboxylic acid esters and lactones, epoxides, phosphate esters, and sulfonic acid esters[3] Chemically, this substance does not have hydrolysable functional groups and hydrolysis is not likely to be a significant fate process if released into the aquatic environment. Therefore, no further testing for this end point is proposed.

5.3 Photodegradation

5.3.1 Summary of Available Data

No published or unpublished photodegradation studies with phenol, heptyl derivatives were located.

5.3.2 Data Assessment and Test Plan for Photodegradation

The Atmospheric Oxidation Potential (AOP) of this substance was characterized using EPA's Quantitative Structure Activity Relationship (QSAR) program, EPIWIN[4]. Atmospheric photooxidation is the degradation of a chemical in air due to reaction with ozone or hydroxyl radicals and is dependent on the chemical structure, concentration and hydroxyl radical concentration. An overall hydroxyl rate constant of 48.8×10^{-12} cm^3/molecule-sec was calculated with a half-life of 2.6 hours. This indicates that atmospheric heptylphenol will be rapidly degraded and will not be persistent.

5.4 Fugacity Modeling

5.4.1 Summary of Available Data

No published or unpublished fugacity-based multimedia fate modeling data for phenol, heptyl derivatives was located.

5.4.2 Test Plan for Fugacity

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[2] Brendshag, et al. Toxicity Testing and chemical characterization of produced water – A preliminary study In Ray JP, Engelhart FR Eds. Produced Water. Technological/Environmental Issues and Solutions. Plenum. New York, NY, USA. Pp 245-260.

[3] Neely, W. B. 1985. Hydrolysis. In: W. B. Neely and G. E. Blau, Eds. Environmental Exposure from Chemicals. Vol I., pp. 157-173. CRC Press, Boca Raton, FL, USA.

[4] Estimation Program Interface for Windows (EPIWIN), Version 3.02. Syracuse Research Corporation, Syracuse, NY.

The relative distribution of phenol, heptyl derivatives among environmental compartments was evaluated using Level I Equilibrium Criterion (EQC) model[5]. Fugacity modeling was conducted using experimentally derived physico-chemical input parameters for vapor pressure, water solubility and octanol-water partition coefficient. The level I model predicts the equilibrium distribution of a fixed quantity of a chemical in a closed environment at equilibrium, with no degrading reaction, advective processes and no intermedia transport. The medium receiving the emission is unimportant because the chemical is assumed to be instantaneously distributed to an equilibrium condition. A Level III fugacity modeling is not appropriate as potential discharge rates into various environmental compartments and the reaction half-life estimates are not known for this chemical.

The Level I modeling results are presented below which indicate the likely environmental compartment into which a chemical will tend to partition and an indication of the distribution in each medium.

Chemical	Air (%)	Water (%)	Soil (%)	Sediment (%)	Sesp. Sediment (%)	Fish (%)
Heptyl Phenol	13.9	2.9	81.4	1.8	0.06	0.0046

6.0 ECOTOXICOLOGY DATA

6.1 Aquatic Toxicity

<u>6.1.1 Summary of Available Data</u>

Heptyl phenol is toxic to fish based on data available in the scientific literature[1]. No data was located for invertebrates or algae.

<u>6.1.2 Data Assessment and Test Plan for Acute Aquatic Ecotoxicity</u>

A 96-hour median lethal concentration of 0.56 mg/L was obtained in a flow through acute toxicity study conducted with juvenile fish, Atlantic cod (*Gadus morhua L.*) Aquatic toxicity testing will be conducted in invertebrates and algae according to OECD Test Guidelines 201 and 202 (Part 1).

7.0 MAMMALIAN TOXICOLOGY DATA

7.1 Acute Mammalian Toxicity

<u>7.1.2 Summary of Available Data</u>

Acute oral and dermal toxicity studies are available for phenol, heptyl derivatives. In these studies, the LD_{50}s are between 0.2g/kg and 2.0g/kg, respectively.

<u>7.1.3 Data Assessment and Test Plan for Acute Mammalian Toxicity</u>

[5] Mackay, D.A et al. Assessing the Fate of New and Existing Chemicals: A Five-Stage Process. Environ. Toxicol. Chem. 15, 1618-1626 (1996).

Adequate and reliable acute oral and dermal toxicity tests were performed for phenol, heptyl derivatives. Additional acute mammalian toxicity testing will not be conducted.

7.2. Mutagenicity

7.2.1 Summary of Mutagenicity Data

An adequate and reliable gene mutation study was performed for phenol, heptyl derivatives. The test substance was not mutagenic in the assay with or without metabolic activation.

7.2.2 Data Assessment and Test Plan for Mutagenicity Toxicity

A chromosomal aberration study will be conducted according to OECD Test Guideline 473.

7.3 Repeated-dose, Reproductive and Developmental Toxicity

7.3.1 Summary of Repeated-Dose Toxicity Data

No published or unpublished repeat dose, reproductive or developmental toxicity tests for phenol, heptyl derivatives were located.

7.3.2 Data Assessment and Test Plan for Repeated-dose Toxicity

A combined repeated dose toxicity study with a reproduction/developmental toxicity-screening test will be conducted according to OECD Test Guideline 422.

8.0 SUMMARY

The following table summarizes the proposed testing on phenol, heptyl derivatives.

Table 1
Summary Table of Available Data and Proposed Testing on Phenol, Heptyl Derivatives

CAS No.: 72624-02-3	Study Results	Testing Proposed
Physical/Chemical Characteristics		
Melting Point	Not Applicable	No
Boiling Point	256 - 280°C	No
Vapor Pressure	0.0113 mm Hg @ 25ºC	No
Water Solubility	12.2 mg/L	No
Partition Coefficient	4.5 experimental	No
Environmental Fate		
Biodegradation	Inherently biodegradable (25% in 28 days)	No
Hydrolysis	Technical discussion included	No
Photodegradation	Modeling results included	No
Fugacity	Modeling results included	No
Ecotoxicity		
Acute Toxicity to Fish	96 hour LC50 = 2.9umol/L	No
Acute Toxicity to Invertebrates	No Data Located	Yes
Acute Toxicity to Algae	No Data Located	Yes
Mammalian Toxicity		
Acute Toxicity	Oral LD_{50} > 0.2 g/kg (rat) Dermal LD_{50} >2.0 g/kg (rabbit)	No
Repeated Dose Toxicity	No Data Located	Yes
Developmental Toxicity	No Data Located	Yes
Reproductive Toxicity	No Data Located	Yes
Genotoxicity		
Gene Mutation	Not Mutagenic	No
Chromosomal Aberration	No Data Located	Yes